Collective Charge Density Wave motion through an ensemble of Aharonov-Bohm rings

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We investigate theoretically the collective charge density wave motion through an ensemble of small disordered Aharonov-Bohm rings. It is shown that the magnetic flux modulates the threshold field and the magnetoresistance with a half flux quantum periodicity $\Phi_0/2 = h/2e$, resulting from ensemble averaging over random scattering phases of multiple rings. The magnitude of the magnetoresistance oscillations decreases rapidly with increasing bias. This is consistent with recent experiments on $NbSe_3$ in presence of columnar defects [Phys. Rev. Lett. **78**, 919 (1997)].

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One of the first experimentally observed quantum phenomena in charge density wave (CDW) compounds is the oscillating magnetoresistance in $NbSe_3$ in presence of small columnar defects, recently reported by Latyshev et al. [1]. The collective response of the CDW to the Aharonov-Bohm flux trapped inside the columnar defects reflected a $\Phi_0/2 = h/2e$ periodicity. The occurrence of this period was related to instantons [2] in ring-shaped commensurate CDW conductors, where large scale quantum fluctuations of the CDW phase allow for macroscopic quantum tunneling between degenerate ground states. Related work [3] on CDW's in a ring geometry, however, predicts a periodicity of Φ_0 due to the modulation of the amplitude of the order parameter. It is doubtful whether these models apply to an array of columnar defects in a planar film. Here we propose a different theoretical model, which is closer related to the actual experimental geometry, and can account for the observed effects.

Figure 1 shows schematically a planar film of one-dimensional CDW chains, containing a small hole threaded by magnetic flux. The CDW is characterized by a complex order parameter $|\Delta| \exp(i\chi)$, where $|\Delta|$ is proportional to the amplitude of the density modulation and the phase χ denotes its position. The size of the hole is smaller than both the longitudinal $\xi_\parallel$ and transversal $\xi_\perp$ CDW coherence lengths. As recently shown by Artemenko and Gleisberg [4], nonlinear screening of the phase distortions induced by a defect, leads to the formation of metallic islands surrounding the latter. Hence, in our model we include a small conducting region around the hole where the CDW order is destroyed. In the normal region, electrons can encircle the hole via different paths, as indicated by the dotted lines, each picking up a random scattering phase. Because of the strong anisotropy, the largest contribution will arise from the middle chains. Therefore, as a model calculation, we proceed with a one-dimensional treatment of the problem.

Using microscopic equations for the sliding CDW motion "over" a general scattering source, we show that the Aharonov-Bohm flux modulates the CDW threshold field. The periodicity $\Phi_0/2$ appears by ensemble averaging over random scattering phases, as is known from the Al'tshuler, Aronov, and Spivak (AAS)-theory [5] for an ensemble of Aharonov-Bohm rings. Our results qualitatively account for the amplitude of the magnetoresistance oscillations and its disappearance at higher bias.

In the framework of the kinetic equations [6], the motion of the quasi-particles and the condensate in a quasi one-dimensional CDW conductor can be described by the semiclassical Green functions $g^i_{\alpha\beta}(x;t,t')$ where $i = \{R, A, K\}$ and $\alpha, \beta = \{1, 2\}$. The retarded $\mathbf{g}^R$ and advanced $\mathbf{g}^A$ functions determine the excitation spectrum and the Keldysh component $\mathbf{g}^K$ describes the kinetics of the system. The subscripts 1 and 2 refer to the right-, respectively, left-moving electrons at the two branches of the linearized energy spectrum. We incorporate the effects of the Aharonov-Bohm ring in this formalism, by imposing boundary conditions on the Green functions.

The Green functions at the right (R) and left (L) of a small scattering source of characteristic length $l < \xi_0$ are related by

$$\mathbf{g}^i_R = (\mathbf{M}^\dagger)^{-1}\mathbf{g}^i_L\mathbf{M}^\dagger, \tag{1}$$

where $\mathbf{M}$ is the transfer matrix of the scatterer which satisfies the condition $\mathbf{M}^{-1} = \boldsymbol{\sigma}_3\mathbf{M}\boldsymbol{\sigma}_3$ in order to ensure current conservation. The transfer matrix $\mathbf{M}$ can generally be paramtrized as

$$\mathbf{M} = \begin{pmatrix} e^{i\eta_0}\sqrt{1+\lambda} & e^{i\varphi_0}\sqrt{\lambda} \\ e^{-i\varphi_0}\sqrt{\lambda} & e^{-i\eta_0}\sqrt{1+\lambda} \end{pmatrix}, \tag{2}$$

where η_0, φ_0 are scattering phases and $\lambda/(1+\lambda) = R$ is the reflection probability of the scatterer [7]. To investigate the motion of the CDW in the vicinity of the scatterer we proceed in five steps. First we gauge away the phase $\chi(x,t)$ of the CDW by performing the unitary transformation

$$\tilde{\mathbf{g}}^i(x;t,t') = \mathbf{U}^\dagger(x,t)\mathbf{g}^i(x;t,t')\mathbf{U}(x,t'), \tag{3}$$

where $\mathbf{U} = \exp\frac{i}{2}\chi\boldsymbol{\sigma}_3$. Then we apply a Fourier transformation with respect to the time difference in Wigner's representation

$$\mathbf{g}^i(x;t-t',T)=\int\frac{d\epsilon}{2\pi}\mathbf{g}^i(x,\epsilon,T)e^{-i\epsilon(t-t')/\hbar}, \tag{4}$$

with $T=(t+t')/2$. The third step is to restrict ourselves to the Keldysh Green function and integrate it over all energies. Using the identity $\int\partial_\epsilon\mathbf{g}^K d\epsilon=4\boldsymbol{\sigma}_3$ we obtain the boundary condition

$$\boldsymbol{\mathcal{L}}\int d\epsilon\tilde{\mathbf{g}}_R^K-\int d\epsilon\tilde{\mathbf{g}}_L^K\boldsymbol{\mathcal{L}}+2\hbar(\dot{\chi}_R-\dot{\chi}_L)\boldsymbol{\mathcal{L}}=0, \tag{5}$$

where $\boldsymbol{\mathcal{L}}=\mathbf{U}_L^\dagger\mathbf{M}^\dagger\mathbf{U}_R$, and $\dot{\chi}_{R,L}=\partial_t\chi_{R,L}$ define the sliding CDW velocities at the right and left side of the scatterer, respectively. Next it is convenient to decompose the matrices into the unit matrix and the three Pauli matrices as $\tilde{\mathbf{g}}=g_0\mathbf{1}+\vec{g}\cdot\vec{\boldsymbol{\sigma}}$ and $\boldsymbol{\mathcal{L}}=\mathcal{L}_0\mathbf{1}+\vec{\mathcal{L}}\cdot\vec{\boldsymbol{\sigma}}$, where $\vec{g}=(g_1,g_2,g_3)$, $\vec{\mathcal{L}}=(\mathcal{L}_1,\mathcal{L}_2,\mathcal{L}_3)$ and $\vec{\boldsymbol{\sigma}}=(\boldsymbol{\sigma}_1,\boldsymbol{\sigma}_2,\boldsymbol{\sigma}_3)$. After substitution into (5) we are left with the equations

$$\int d\epsilon(g_{0,R}^K-g_{0,L}^K)+2\hbar(\dot{\chi}_R-\dot{\chi}_L)=0 \tag{6a}$$

$$\mathcal{L}_0\int d\epsilon(\vec{g}_R^K-\vec{g}_L^K)+i\vec{\mathcal{L}}\times\int d\epsilon(\vec{g}_R^K+\vec{g}_L^K)=0. \tag{6b}$$

From the defenition of current

$$-I=\frac{eN(0)v_F}{4}\int d\epsilon\mathrm{Tr}\tilde{\mathbf{g}}^K+eN(0)v_F\hbar\dot{\chi}, \tag{7}$$

where $-e$ is the electron charge, v_F is the Fermi velocity and $N(0)$ is the density of states at the Fermi energy, it is seen that the first equation just expresses the conservation of current through the scatterer. In the quasi-stationary approximation, where we neglect the inertia of the CDW ($\partial_t^2\chi=0$) and the time dependence of the amplitude of the order parameter, we know from the self-consistency equation that

$$\int d\epsilon g_1^K=0,\quad\int d\epsilon g_2^K=-i\frac{|\Delta|}{\gamma}, \tag{8}$$

where γ is the dimensionless electron-phonon coupling constant [8]. Substituting Eqs. (2) and (8) into Eq. (6b), we finally obtain

$$\chi_R-\chi_L=2\eta_0, \tag{9a}$$

$$\mu_R-\mu_L-\frac{|\Delta|}{2\gamma}\sqrt{R}\cos(\chi-\varphi_0)=0. \tag{9b}$$

Here we have defined the electrochemical potential $4\mu=-\int d\epsilon g_3^K$, $\chi=(\chi_R+\chi_L)/2$, and we have assumed equal amplitudes of the CDW order parameter at the right and left contacts $|\Delta|_R=|\Delta|_L=|\Delta|$. The first equation represents the correlation between the CDW's on the right and left hand side of the scatterer in equilibrium, and is necessary for a self-consistent treatment of pinning. The second equation is the desired equation of motion for the CDW. It is similar to the phenomenological single particle model for impurity pinning [9] with threshold potential μ_T given by $\mu_T=|\Delta|\sqrt{R}/2\gamma$. Equation (9b) allows us to calculate the conductance of a CDW moving over a small-size but arbitrary scattering source, which is characterized by its transfer matrix evaluated at the Fermi energy.

Now that we have studied the problem of a general scatterer we proceed by calculating the transfer matrix of a disordered ring threaded by a Aharonov-Bohm magnetic flux. Following Büttiker [10], the two junctions of the ring are described by the unitary scattering matrix $\mathbf{S}$, which relates the outgoing to the incoming scattering amplitudes

$$\mathbf{S}=-\frac{1}{2}\begin{pmatrix}\Omega_--\Omega_+ & \sqrt{\beta} & \sqrt{\beta}\\ \sqrt{\beta} & -\Omega_- & \Omega_+\\ \sqrt{\beta} & \Omega_+ & -\Omega_-\end{pmatrix}, \tag{10}$$

where $\Omega_\pm=1\pm\sqrt{1-2\beta}$, and $0\le\beta\le\frac{1}{2}$ is a coupling parameter describing the reflection at the entrance. We represent the upper $(+)$ and lower $(-)$ path around the ring with the transfer matrices $\mathbf{N}_+$ and $\mathbf{N}_-$, parametrized as

$$\mathbf{N}_\pm=\begin{pmatrix}e^{i\eta_\pm} & 0\\ 0 & e^{-i\eta_\pm}\end{pmatrix}, \tag{11}$$

where $\eta_\pm$ and $\phi_\pm$ are the scattering phases of the separate branches. For simplicity we consider here the clean limit without barriers in both arms, and associate only different scattering phases to different paths. A more general analysis will be presented elsewhere [11]. The phase shift of the electrons due to the magnetic flux is accounted for by the transformation $\mathbf{N}_\pm\to\exp(\pm i\vartheta)\mathbf{N}_\pm$, where $\vartheta=\pi\Phi/\Phi_0$ with flux quantum $\Phi_0=h/e$. After some algebra we obtain the total transfer matrix $\mathbf{M}$ of the disordered ring

$$\begin{aligned}\Lambda M_{11}&=\Omega_-^2\cos2\phi+\Omega_+^2\cos2\vartheta\\&\quad-4(1-\beta)\cos2\eta-4i\beta\sin2\eta\\ \Lambda M_{22}&=-(\Lambda M_{11})^*\\ \Lambda M_{12}&=-\Lambda M_{21}=\Omega_-^2\cos2\phi\\&\quad-\Omega_+^2\cos2\vartheta+4\sqrt{1-2\beta}\cos2\eta,\end{aligned} \tag{12}$$

where we have defined $\eta=(\eta_++\eta_-)/2$, $\phi=(\eta_+-\eta_-)/2$ and $\Lambda=4\beta\{\exp(i\eta)\cos(\vartheta+\phi)-\exp(-i\eta)\cos(\vartheta-\phi)\}$. It is easily verified that this transfer matrix ensures current conservation. From Eq. (6b) we obtain $\varphi_0=\pi/2$ and the self-consistency relation becomes

$$\chi_R-\chi_L=2\arctan\left(\frac{1-\beta}{\beta}\tan\eta-\frac{\Omega_+^2\sin^2\vartheta+\Omega_-^2\sin^2\phi}{2\beta\sin2\eta}\right), \tag{13}$$

which oscillates as a function of the flux and the scattering phases η and ϕ. The threshold field also depends

strongly on the magnetic flux and the scattering phases through

$$\mu_T(\Phi,\eta,\phi) = \left|\frac{M_{21}}{M_{22}}\right| \frac{|\Delta|}{2\gamma}. \tag{14}$$

This expression is dominantly periodic in the flux quantum, but also contains higher harmonics from weak-localization paths. As expected for equal phases $\phi = 0$, destructive interference at values $\Phi = \Phi_0/2 \mod \Phi_0$ enhances the total backscattering and thus the pinning force. For $\phi \neq 0$ its behavior is more complex.

So far we considered only a single Aharonov-Bohm ring. We now turn to the problem of an ensemble of rings in a CDW system. It is well known that the resistance of an ensemble of Aharonov-Bohm rings in series or parallel retains only the half flux quantum periodicity $\Phi_0/2$ [5,12]. This is due to the different scattering phases of subsequent rings. Interference effects of electrons traveling only half the ring circumference average out. However, if electrons encircle the rings just once, the phase difference of time-reversed paths is $\Phi_0/2$ independent of the scattering properties of the individual rings. In our model the ensemble average comes about from averaging over multiple columnar defects. In the limit of strong pinning where $\sqrt{R}|\Delta|/(\pi\hbar v_F n) \gg 1$, with large impurity potentials or a low impurity concentration n, it is known from the Fukuyama-Lee-Rice (FLR) model [13] that the CDW adjust its phase to each defect in order to minimize the electrostatic Coulomb energy. As a consequence the net threshold field is proportional to the sum over all impurities. For uncorrelated defects in series the above formalism reproduces the FLR-model in this limit. If we assume a random distribution of scattering phases for the Aharanov-Bohm rings, we obtain the net threshold field E_T by taking the ensemble average over the scattering phases η and ϕ of a single hole

$$E_T(\Phi) = \frac{1}{4\pi^2 ed} \int_{-\pi}^{\pi} d\eta \int_{-\pi}^{\pi} d\phi\, \mu_T(\Phi,\eta,\phi), \tag{15}$$

where d is the average distance between the columnar defects. The result is shown in Fig. 2 for different values of the parameter β. The average threshold field oscillates as a function of half the flux quantum $\Phi_0/2$ around a constant value. With increasing reflection β at the junctions the total threshold shifts upwards and higher harmonics become visible due to the increasing dwell-time of electrons in the rings. The appearance of a finite pinning force at zero field arising from the columnar defects is consistent with experiments.

Above we have shown that the threshold field of an ensemble of columnar defects oscillates with a half flux quantum period. To qualitatively understand the effect of the flux dependent threshold field on the current-voltage characteristics, we distinguish between the high and low sliding velocity regimes. Near threshold the depinning and dynamics of CDW's can be described as a dynamical critical phenomenon [14]. The CDW current I_{CDW} obeys the scaling relation

$$I_{CDW} \propto \left(\frac{E - E_T}{E_T}\right)^{\alpha}, \tag{16}$$

where the critical exponent α takes the value 3/2 in mean-field [15]. Since the threshold field contains a flux-dependent term as in Eq. (15), large oscillations in the magnetoresistance are expected with $\Phi_0/2$ periodicity. In the high velocity limit, however, the magnetoresistance oscillations disappear rapidly, since the CDW does not see the pinning potentials and their flux dependence. We remark that if we are allowed to neglect phase-slip processes, the potential drop over a single defect should be smaller than the gap $|\Delta|$. The actual correlation between the phases left and right is probably smaller that in our model calculation, due to, for example, the finite size of the hole and the metallic region. If we take into account the energy dependence of the transfer matrix, it can be shown that the pinning force in Eq. (9b) is then modified by $|\Delta| \to |\Delta| \exp(-l/\xi_0)$.

In comparison with the experiments [1], this model accounts for the periodicity of the magnetoresistance oscillations and qualitatively for the decrease of the amplitude at large biases. The observed minimum at zero field may arise from spin-orbit interaction, which is known to determine the sign of the magnetoresistance oscillations in compounds with relatively large atomic-numbers [5]. This has not been taken into account presently and needs further investigation as well as an extension to multiple channels. Experimentally, measurements of the dependence of the threshold field on the magnetic flux should provide more insights into the validity of our model.

We conclude by summarizing our results. We have derived microscopic equations for the non-linear sliding CDW motion over an arbitrary scatterer. It is shown that magnetic flux trapped in a columnar defect modulates the threshold field. In a low density ensemble of defects, averaging results in a half flux quantum periodicity of the magnetoresistance. The amplitude of oscillation decreases rapidly with increasing bias.

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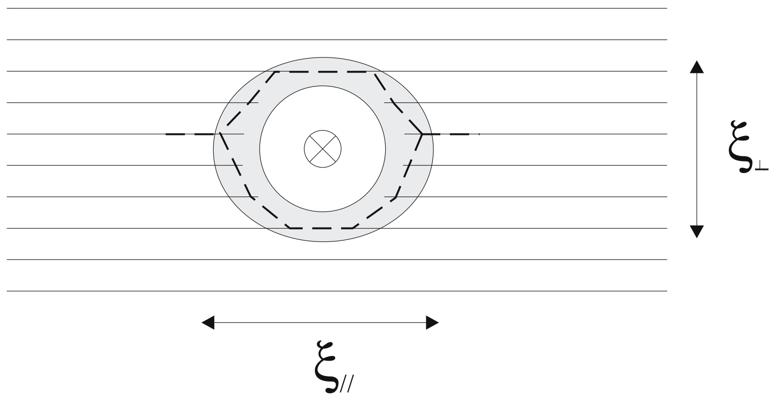
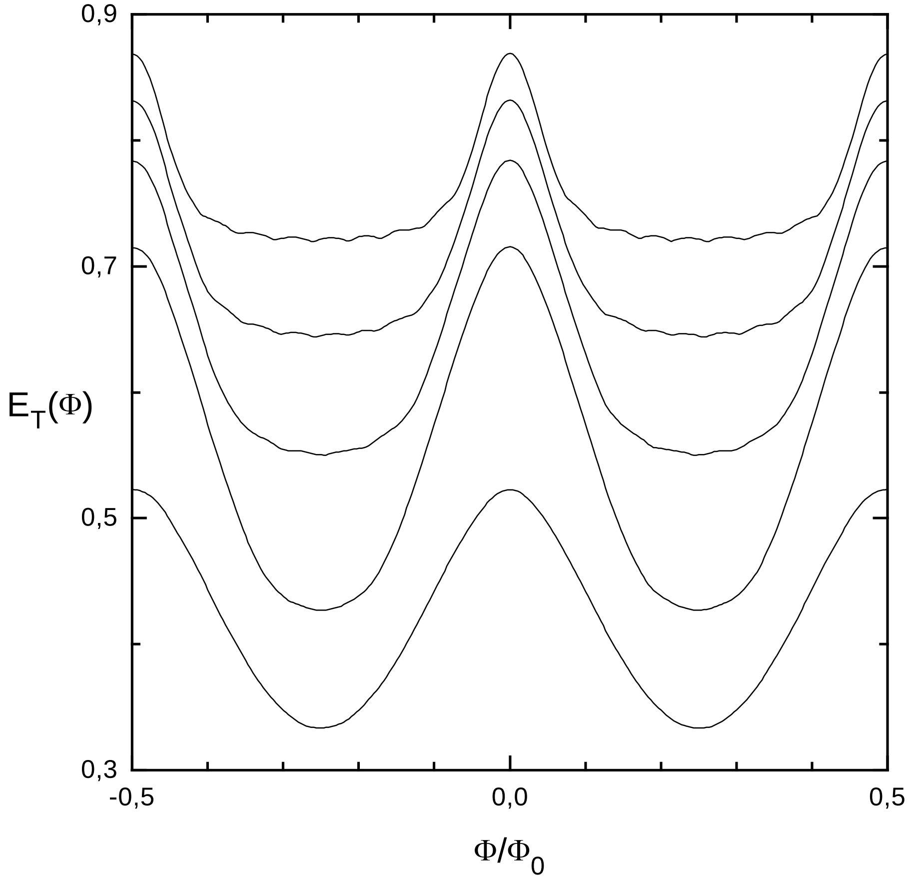
FIG. 1. Schematic figure of a small columnar defect threaded by magnetic flux in a planar film of CDW chains. Electrons can encircle the hole through a metallic region, where the CDW order is assumed to be destroyed (shaded area).

FIG. 2. Averaged threshold field E_T in units of $|\Delta|/2\gamma ed$ as a function of magnetic flux for different values of $\beta = 0.3; 0.35; 0.4; 0.45; 0.5$ from top to bottom.



$\xi_{\perp}$
$\xi_{//}$


0,9
0,7
0,5
0,3
E_T(Φ)
-0,5
0,0
0,5
Φ/Φ_0